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13. ABSTRACT (Maximum 200 words) A number of improvements to PDEPACK have been made. These include the development of parallel discretization methodologies and sparse/iterative PDE solvers.				
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FINAL REPORT FOR AFOSR CONTRACT F49620-92-J-0069
High Performance Computing Methods and Systems for Partial Differential
Equations

Period September 1, 1992 - February 28, 1995

July 19, 1995

A. PROJECT RESULTS

In this report we list the personnel that worked under this AFOSR grant, the publications completed and describe the accomplishments of various projects. The results under this contract include:

PDEPACK: The PDE solving system PDEPACK has been designed and a prototype made operational. Its objectives are

- Provide a software framework for PDE solving,
- Integrate major public domain PDE solvers and libraries,
- develop parallel discretization methodologies and sparse/iterative solvers.

The status of the software in PDEPACK is as follows:

Already Incorporated

ELLPACK	MGGAT
//ELLPACK	PATRAN
FIDISOL	PCGPACK
VECFEM	PDECOL
NSPCG	PDEONE
Sparskit	LINPACK
CVD RCTR	VERSE
CADSOL	CFD

In Process of Being Incorporated

PTS
PDETWO
OCEAN
MP PCGPACK2

Being Studied for Incorporation

LAPACK
ACM Algorithms 392,494,533,572,593,651
IMSL
DLEARN

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PDELab: PDEPACK is the basis for PDELab, a problem solving environment for high performance PDE applications. Its objectives are

- A generic environment to specify PDE models,
- A unified interactive PDE solving environment,
- Assistance in making decisions at all levels of PDE solving.

The software architecture for PDELab has been completed and a prototype is operational. PDELab is a general problem solving environment for high performance PDE based applications; it is based on the solvers in PDEPACK. Two application specific problem solving environments have been designed to be built on top of PDELab. One, called BioSeparation Lab, is operational. It incorporates a PDE model of the chemical engineering process along with online connections to actual experimental apparatus so the process can be controlled. The second one is still being built; it is to model and control the Chemical Vapor Deposition process used to make microchip wafers.

PYTHIA: The PDELab prototype incorporates the expert system *PYTHIA* which

- Uses exemplar and neuro-fuzzy based learning to guide the selection of software and hardware for PDE applications.
- Has a knowledge base facility that automatically generates value to support "smart" sequential and parallel PDE solvers.

WWW Servers: A prototype World Wide Web based server for PDELab has been designed and is operational. It allows a user on the internet to solve elliptic PDEs using //ELLPACK (a subset of PDELab) on our server and its associated parallel machines. This system is being enhanced and extended for all of PDELab.

Basic Research: A variety of more basic research results have been obtained to:

- Analyze the performance of parallel computation
- Analyze numerical methods for partial differential equations
- Analyze the partitioning of PDE problems for parallel computation.

B. PERSONNEL

Work on this grant has involved the following people:

John R. Rice*(Co-PI)	Professor of Computer Science
Elias N. Houstis*(Co-PI)	Professor of Computer Science
Apostolos Hadjidimos*	Visiting Professor of Computer Science
Catherine E. Houstis	Visiting Assoc. Professor of Computer Science
Cheryl Crabill*	Programmer
Manolis Vavalis*	Postdoc
Mo Mu*	Postdoc
Ko Yang Wang*	Postdoc
Nicholas Chrisochoides*	Ph.D. candidate
Sanjiva Weerawarana*	Ph.D. candidate
Sang Bae Kim	Ph.D. candidate
Scott McFadden	Ph.D. candidate
Hyeran Byun	Ph.D. candidate
Yu-Ling Lai	Ph.D. candidate
Po-Ting Wu	Ph.D. candidate
Mei-Ling Shyu*	Ph.D. candidate
Chi Chui*	Ph.D. candidate
Winnie Lap-kan Ng*	Ph.D. candidate
Pelayia Varodoglu	M.S. student
Jim Berniger*	M.S. student
Athanasios Gaitatzes	M.S. student
Margaret Gaitatzes	M.S. student, Programmer
Shahani Weerawarana	M.S. student
Hongtao Gu*	M.S. student
Konstantios Pantazopoulos*	M.S. student
Jeffrey Michael*	M.S. student
Meletis Samartzis*	Visiting Research Associate
Stavros Kortesis	Visiting Scholar

Those names with stars have received some direct AFOSR support, the others have research support from related projects.

C. EXTERNAL HONORS

John R. Rice

- *ACM Service Award*: Assoc. Comp. Mach., March 1993.
- *CRA Service and Leadership Award*: Computing Research Assoc., July 1993.
- Elected to National Academy of Engineering, 1994.
- Sigma Xi Award for Outstanding Research by Purdue Faculty Member, 1994.
- Appointed to editorial board of IEEE Computational Science and Engineering, 1994.

- Appointed Academic Advisory Board of Industrial Research Institute, 1995.

D. PUBLICATIONS

We list the publications that have resulted from the past three years of work supported by the AFOSR. These include:

- 13 Journal papers
- 3 Papers submitted for journal publication
- 14 Refereed Conference papers
- 1 Book edited
- 1 Ph.D. Thesis
- 7 Papers in books/proceedings

1. REFEREED JOURNALS

1. H.S. McFadden and J.R. Rice, Collaborating PDE solvers. *Applied Numerical Mathematics*, **10**, (1992), 279–295.
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3. A. Hadjidimos, E.N. Houstis, E.A. Vavalis, and J.R. Rice, Iterative line cubic spline collocation methods for elliptic partial differential equations in several dimensions. *SIAM J. Sci. Stat. Comp.*, **14** (1993), 715–734.
4. M. Mu and J.R. Rice, An organization of sparse Gauss elimination for solving partial differential equations on distributed memory machines. *Numer. Meth. Part. Diff. Eqns.*, **9** (1993), 175–189.
5. D.C. Marinescu and J.R. Rice, On high level characterization of parallelism. *J. Par. Dist. Comp.*, **20** (1994), 107–113.
6. M. Mu and J.R. Rice, Preconditioning for domain decomposition through functional approximation. *SIAM J. Sci. Comp.*, **15** (1994), 1452–1466.
7. N. Chrisochoides, E.N. Houstis, and J.R. Rice, Mapping algorithms and software environments for data parallel PDE iterative solvers. *J. Par. Dist. Comp.*, **21**, (1994), 75–95.
8. Y.-L. Lai, A. Hadjidimos, E.N. Houstis, and J.R. Rice, General interior hermite collocation methods for second order elliptic partial differential equations. *Applied Numerical Methods*, (1995), to appear.

9. D.C. Marinescu, J.R. Rice, and E.A. Vavaliş, Performance of iterative methods for distributed memory machines. *Applied Numerical Mathematics*, **12** (1994), pp. 421–430. Extended abstract in *Proc. 13th World Congress, IMACS*, Rutgers University, New Brunswick, NJ, Vol. 2 (1991), 684–685.
10. D.C. Marinescu and J.R. Rice, On the scalability of asynchronous parallel computations. *J. Par. Dist. Comp.*, **22** (1994), 538–546.
11. E. Gallopoulos, E.N. Houstis, and J.R. Rice, Computer as thinker/doer: Problem solving environments for computational science. *IEEE Comp. Sci. Engr.*, **1** (1994), 11–23.
12. J. Lambers and J.R. Rice, QUAD2D: Adaptive quadrature for general two dimensional domains, submitted as paper and companion algorithm.
13. S.B. Kim, A. Hadjidimos, E.N. Houstis, and J.R. Rice, Multi-parameterized Schwarz splittings, submitted to *Numerical Linear Algebra and Applications*.
14. A. Hadjidimos and D. Noutsos, On a matrix identity connecting iteration operations associated with a p-cyclic matrix, *Linear Algebra Appl.*, **182** (1993), 157–177.
15. A. Hadjidimos and M. Neumann, On domains of superior convergence of the SSOR method over the SOR method, *Linear Algebra Appl.*, **187** (1993), 67–85.
16. M. Mu and J.R. Rice, Modeling with collaborating PDE solvers – Theory and practice. *Contemporary Mathematics*, **180**, (1994), 427–438.

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17. A. Hadjidimos and R.J. Plemmons, Analysis of p-cyclic iterations for Markov chains, in *Linear Algebra, Markov Chains, and Queueing Models*, (C.D. Meyer and R.J. Plemmons, eds.), IMA Series on Applied Mathematics, Springer-Verlag, **48** (1993), 111–124.
18. M. Mu and J.R. Rice, A PDE sparse solver benchmark for massively parallel distributed memory multiprocessors. In *Computer Methods for Partial Differential Equations VII* (R. Vichnevetsky, ed.), IMACS, New Brunswick, NJ (1992), 546–552.
19. E.N. Houstis and J.R. Rice, The architecture of PDE solving systems. In *Computer Methods for Partial Differential Equations VII* (R. Vichnevetsky, ed.), IMACS, New Brunswick, NJ (1992), 363–370.
20. N. Chrisochoides, E.N. Houstis, S.B. Kim, M.K. Samartzis, and J.R. Rice, Parallel iterative methods. In *Computer Methods for Partial Differential Equations VII* (R. Vichnevetsky, ed.), IMACS, New Brunswick, NJ (1992), 134–141.

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25. A. Catlin, C. Chui, C. Crabill, E.N. Houstis, S. Markus, J.R. Rice, and S. Weerawarana, PDELab: An object-oriented framework for building problem solving environments for PDE based applications, submitted to a conference.
26. P. Wu, E.N. Houstis, and J.R. Rice, EPPOD: A parallel problem solving environment for the electronic prototyping of physical objects design, *Proc. DAGS '94 Symposium*, (F. Makedon, ed.), Dartmouth Inst. Adv. Grad. Studies, Dartmouth, NH (1994), 135-151.
27. E.N. Houstis, S. Weerawarana, A. Joshi, and J.R. Rice, The PYTHIA project, *First Intl. Conf. on Neural, Parallel and Scientific Computations*, 1995.
28. A. Joshi, S. Weerawarana, and E.N. Houstis, Using neural networks to support intelligent scientific computing, *Proceedings IEEE Intl. Conf. Neural Networks*, Orlando, 1995.
29. A. Joshi, T. Drashansky, E.N. Houstis, S. Weerawarana, SciencePad: An intelligent electronic notepad for ubiquitous scientific computing, *IASTED/ISMM International Conference on Intelligent Information Management Systems*, June 1995, Washington, D.C.
30. P. Wu and E.N. Houstis, A parallel mesh generation and decomposition methodology, *Proceedings of Mesh Generation Conference*, Albuquerque, October 1994.

3. BOOKS, BOOK CHAPTERS, AND PUBLICATIONS IN BOOKS/PROCEEDINGS

3.A. Books

31. E.N. Houstis and J.R. Rice, *Artificial Intelligence, Expert Systems and Symbolic Computing*, North-Holland, Amsterdam (1992).
32. S. Weerawarana, *Problem Solving Environments for Partial Differential Equation Based Systems*, Ph.D. Thesis, Department of Computer Sciences, Purdue University, 1994.

3.B. Publications in Books and Proceedings

33. P. Wu, E.N. Houstis, and J.R. Rice, Geometry as a basis for parallel analysis and design of physical objects, *Second U.S. National Congress on Computational Mechanics* (A.N. Noor, ed.), 1993.
34. R. Sharma and J.R. Rice, Numerical technique to solve nonlinear elliptic PDE's arising from semiconductor device modeling, *Proc. Intl. Workshop on Computational Electronics*, Beckman Inst., Univ. Illinois (1992), 123-126.
35. M. Mu and J.R. Rice, Preconditioner construction with rational approximation. In *Parallel Processing for Scientific Computing. II* (Sinovec, et. al., eds), SIAM Pub., Philadelphia (1993), 678-682.
36. E.N. Houstis, J.R. Rice, and S. Weerawarana, An open structure of PDE solving systems, *Proc. 14th IMACS World Congress*, IMACS 3 (1994), 1296-1299.
37. M.A. Corena-Hasegan, C. Costian, D.C. Marinescu, I. Martin, and J.R. Rice, Towards problem solving environments for high performance computing, *High Performance Computing Conference '94*, Nat. Supercomputer Res. Ctr., Singapore (1994), 354-366.
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